## **Diffusion Processes in Molten Semiconductors**

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## <u>Description of Experiment</u>

For the First Materials Science Laboratory (MSL-1) mission flight of opportunity, this program of study was directed at the fundamental and applied issues pertaining to diffusion of mass in the liquid state as driven by concentration gradients (Fickian diffusion). The fundamental material systems of interest for the MSL-1 mission were the dilute binary systems of gallium (Ga), silicon (Si), and antimony (Sb) into germanium (Ge). This research program consisted of three major components: an experimental measurement portion, a continuum numerical simulation portion, and an atomistic numerical simulation portion.

The experimental measurement portion was designed to provide definitive measurements of the purely diffusive component of mass transfer in molten semiconductor systems. The shear cell technique was used to directly measure the diffusion coefficients in semiconductor melts. For the Fickian diffusion case, isothermal measurements were used to determine the diffusion coefficients. An experimental matrix was used to determine the dependence of the diffusion coefficients on temperature, dopant type, and column diameter. For the MSL-1 mission, the experiments contained a "check" to quantify, if any, the amount of Soret diffusion driven by the small thermal gradients in the Large Isothermal Furnace (LIF).

The shear cell technique consisted of two columns of different liquids which were brought into contact with one another, allowed to diffuse, and then these columns were sheared into segments. Following solidification, the average concentration level of each segment will be measured, enabling the construction of a diffusion profile. From that concentration profile, the diffusion coefficients can be computed and possible diffusion mechanisms may be verified.

## Justification of the Need for Space Environment

Terrestrial experiments designed to measure diffusion coefficients in the liquid state are hampered by convection in the melt and convection during the solidification process, both of which typically confound data interpretation. This has resulted in wide variations in the few reported data in the literature. Arnold and Matthiesen have predicted, based on numerical simulations, that for the Gadoped Ge system, convection effects increase the measured diffusion coefficient and are expected for capillary diameters greater than 2 mm and may be present for capillary diameters less than 2 mm. The experimental data combined with the numerical simulations of convective effects predict a nonexistent range of capillary diameters that allow the measurement of the actual diffusion coefficient on Earth. As a result, the microgravity environment, in which convective effects are minimized, is required.

## **Summary of Results**

Six cartridges were processed on the reflight of the MSL-1 (MSL-1R) Spacelab mission using the National Space Development Agency (NASDA) provided LIF furnace. Each of these cartridges contained one shear cell. The active region of each shear cell consisted of 14 segments which were each 6 mm in length. Two cartridges were processed at 1000 °C, three at 1550 °C, and one at 955 °C.

Each cartridge contained six capillaries, three at 3.0 mm diameter and three at 1.5 mm diameter. In addition there were six 1.0 mm diameter capillaries with five active segments each, which were used as a check to determine if Soret diffusion was present. The material was gallium doped germanium in two sets of the capillaries and antimony doped germanium in one set of capillaries. In the 1000 °C samples, one of the gallium doped germanium columns was co-doped with silicon.

Several anomalies occurred during the MSL-1R mission; however, the integrity of the shear cell appears to have been maintained in all experiments.